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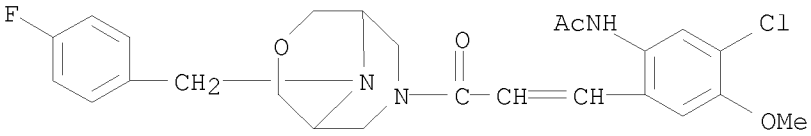
L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 2006:1199252 CAPLUS
DOCUMENT NUMBER: 146:176166
TITLE: Bridged piperazines and piperidines as CCR1 antagonists with oral activity in models of arthritis and multiple sclerosis
AUTHOR(S): Revesz, Laszlo; Bollbuck, Birgit; Buhl, Thomas; Dawson, Janet; Feifel, Roland; Heng, Richard; Hiestand, Peter; Sparrer, Helmut; Schlapbach, Achim; Waelchli, Rudolf; Loetscher, Pius
CORPORATE SOURCE: Global Discovery Chemistry, Novartis Institutes for BioMedical Research, Basel, CH-4002, Switz.
SOURCE: Letters in Drug Design & Discovery (2006), 3(10), 689-694
CODEN: LDDDAW; ISSN: 1570-1808
PUBLISHER: Bentham Science Publishers Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

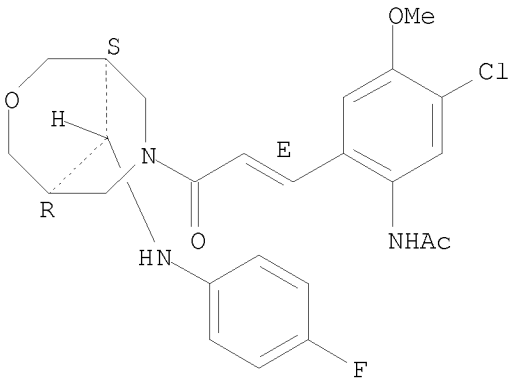
AB CCR1 antagonists were prepared by coupling bridged piperazines and bridged piperidines with 2-acetylamino-4-chloro-5-methoxy cinnamic acid. Compound 2 of the series showed the desired equal potency against human, mouse and rat CCR1 (IC50 = 20; 22; 28 nM), exhibited a superior pharmacokinetic profile and inhibited the clin. grades in rat acute exptl. autoimmune encephalomyelitis and knee swelling in rat antigen induced arthritis at doses of 2 + 30 and 2 + 15 mg/kg p.o.

IT 921208-19-7
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(bridged piperazines and piperidines as CCR1 antagonists with oral activity in models of arthritis and multiple sclerosis)
RN 921208-19-7 CAPLUS
CN Acetamide, N-[5-chloro-2-[3-[9-[(4-fluorophenyl)methyl]-3-oxa-7,9-diazabicyclo[3.3.1]non-7-yl]-3-oxo-1-propen-1-yl]-4-methoxyphenyl]- (CA INDEX NAME)



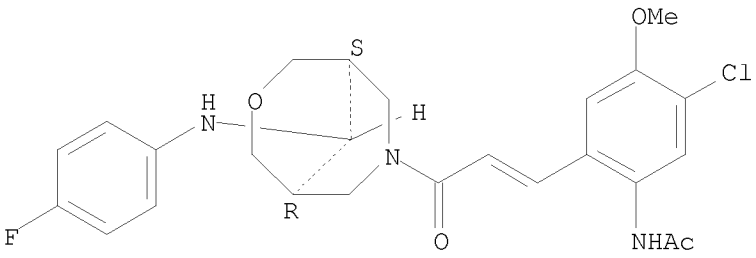
IT 868408-72-4 921208-29-9
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(bridged piperazines and piperidines as CCR1 antagonists with oral activity in models of arthritis and multiple sclerosis)
RN 868408-72-4 CAPLUS
CN Acetamide, N-[5-chloro-2-[(1E)-3-[(9-anti)-9-[(4-fluorophenyl)amino]-3-oxa-7-azabicyclo[3.3.1]non-7-yl]-3-oxo-1-propen-1-yl]-4-methoxyphenyl]- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



RN 921208-29-9 CAPLUS
CN Acetamide, N-[5-chloro-2-[3-[(9-syn)-9-[(4-fluorophenyl)amino]-3-oxa-7-azabicyclo[3.3.1]non-7-yl]-3-oxo-1-propen-1-yl]-4-methoxyphenyl]- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.



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REFERENCE COUNT:	12	THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 2005:1170489 CAPLUS
DOCUMENT NUMBER: 143:440438
TITLE: Preparation of bicyclic heterocycles as CCR-1 and MIP1α antagonists useful against inflammatory diseases and as radiolabeled markers for neuroimaging
INVENTOR(S): Heng, Richard; Revesz, Laszlo; Schlapbach, Achim; Waelchli, Rudolf
PATENT ASSIGNEE(S): Novartis AG, Switz.; Novartis Pharma GmbH
SOURCE: PCT Int. Appl., 205 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005103054	A2	20051103	WO 2005-EP4422	20050425
WO 2005103054	A3	20070208		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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AU 2005235724	B2	20081030		
CA 2559917	A1	20051103	CA 2005-2559917	20050425
AR 52397	A1	20070321	AR 2005-101623	20050425
EP 1794164	A2	20070613	EP 2005-737794	20050425
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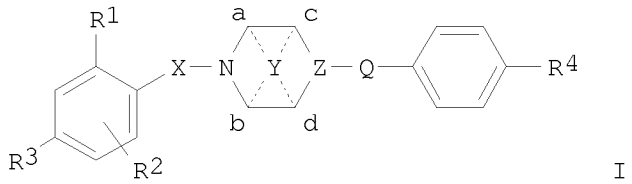
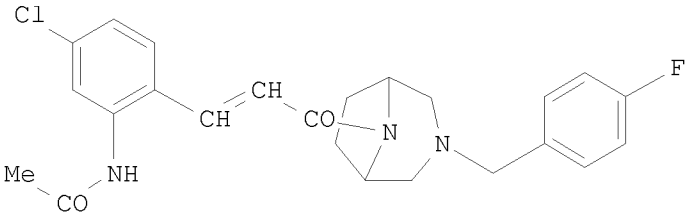
BR 2005010313	A	20071016	BR 2005-10313	20050425
JP 2007534678	T	20071129	JP 2007-508868	20050425
RU 2383548	C2	20100310	RU 2006-141702	20050425
US 20070196270	A1	20070823	US 2006-599819	20061011
KR 2007014154	A	20070131	KR 2006-7022181	20061025
KR 845356	B1	20080709		
MX 2006012380	A	20070117	MX 2006-12380	20061026
IN 2006CN03917	A	20070615	IN 2006-CN3917	20061026
CN 101238131	A	20080806	CN 2005-80013239	20061026
KR 2008015151	A	20080218	KR 2008-7002184	20080128

PRIORITY APPLN. INFO.:	GB 2004-9236	A	20040426
	WO 2005-EP4422	W	20050425
	KR 2006-7022181	A3	20061025

OTHER SOURCE(S): CASREACT 143:440438; MARPAT 143:440438
GI



I



II

AB Bicyclic heterocycles (shown as I; variables defined below; e.g. (E)-N-[5-Chloro-2-[3-[3-(4-fluorobenzyl)-3,8-diazabicyclo[3.2.1]oct-8-yl]-3-oxopropenyl]phenyl]ethanamide (shown as II)) or a pharmaceutically acceptable salt or ester thereof, were prepared and found to be antagonists of CCR-1 and MIP1α and claimed useful for treatment of diseases and conditions in which CCR-11 is implicated, e.g. inflammatory diseases. Compds. I are also claimed useful as radiolabeled markers for neuroimaging, e.g. for diagnosis of Alzheimer's disease. Methods of preparation are claimed and .apprx.160 example prepns. are included. For example, II was prepared in 6 steps (94, 87, 46, 68, 100 and 56 % yields) starting from (E)-3-(2-amino-4-chlorophenyl)-2-propenoic acid Me ester and involving intermediates (E)-3-[2-[(tert-butoxycarbonyl)amino]-4-chlorophenyl]-2-propenoic acid Me ester, (E)-3-[2-[(tert-butoxycarbonyl)amino]-4-chlorophenyl]-2-propenoic acid, 3-(4-fluorobenzyl)-3,8-diazabicyclo[3.2.1]octane/8-(4-fluorobenzyl)-3,8-diazabicyclo[3.2.1]octane, (E)-[5-chloro-2-[3-[3-(4-fluorobenzyl)-3,8-diazabicyclo[3.2.1]oct-8-yl]-3-oxopropenyl]phenyl]carbamic acid tert-Bu ester, and (E)-3-(2-amino-4-chlorophenyl)-1-[3-(4-fluorobenzyl)-3,8-diazabicyclo[3.2.1]oct-8-yl]prop-2-enone. For I: R1, R2 and R3 = H, cyano, halo, nitro or (un)substituted oxy, C1-7 alkyl, C2-7 alkenyl, C2-7 alkynyl, carbonyl, amino, S, cycloalkyl, heterocycloalkyl, aryl, heteroaryl or a substituent forming a bicyclic ring system of which the Ph ring to which it is attached forms part of the bicycle for example butadiene forming naphthyl, or heterobutadiene forming quinolinyl, quinoxalinyl or isoquinolinyl. R4 = H, cyano, halo, nitro or (un)substituted oxy, C1-7 alkyl, C2-7 alkenyl, C2-7 alkynyl, carbonyl, amino, S, cycloalkyl, heterocycloalkyl, aryl, heteroaryl or a substituent forming a bicyclic ring system of which the Ph ring to which it is attached forms part of the bicycle for example butadiene forming naphthyl, or heterobutadiene forming quinolinyl, quinoxalinyl or isoquinolinyl. X is -CH:CHCO-; Y is -(CH2)n- where n = 1-6, -CH2OCH2- or -CH2NRCH2- and is bonded to two of the ring C atoms, bonding being to either the ring C atoms a and b or the ring C atoms c and d; wherein R = H, (un)substituted: C1-7 alkyl, carbonyl, acyl, acetyl or sulfonyl; Z is N or CH-; Q is -CH2-, -NH- or -O-; addnl. details including provisos are given in the claims.

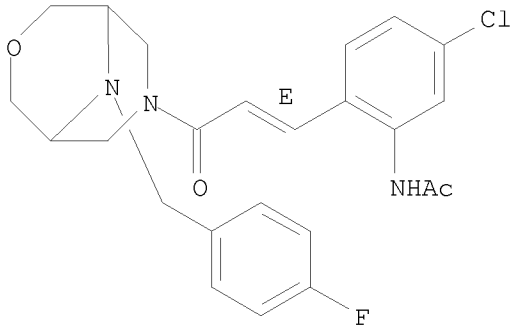
IT 868408-11-1P, (E)-N-[5-Chloro-2-[3-[9-(4-fluorobenzyl)-3-oxa-7,9-diazabicyclo[3.3.1]non-7-yl]-3-oxopropenyl]phenyl]ethanamide
868408-19-9P, (E)-[5-Chloro-2-[3-[9-(4-fluorobenzyl)-3-oxa-7,9-diazabicyclo[3.3.1]non-7-yl]-3-oxopropenyl]phenyl]urea

868408-20-2P, N-[5-Chloro-2-[(E)-3-[9-(4-fluorobenzyl)-3-oxa-7,9-diazabicyclo[3.3.1]non-7-yl]-3-oxopropenyl]-4-methoxyphenyl]acetamide
868408-27-9P, N-[3-Chloro-6-[(E)-3-[9-(4-fluorobenzyl)-3-oxa-7,9-diazabicyclo[3.3.1]non-7-yl]-3-oxopropenyl]-2,4-dimethoxyphenyl]acetamide
868408-28-0P, N-[3-Chloro-6-[(E)-3-[9-(4-fluorobenzyl)-3-oxa-7,9-diazabicyclo[3.3.1]non-7-yl]-3-oxopropenyl]-2-methoxyphenyl]acetamide
868408-29-1P, N-[5-Chloro-2-[(E)-3-[9-(4-fluorobenzyl)-3-oxa-7,9-diazabicyclo[3.3.1]non-7-yl]-3-oxopropenyl]-4-methoxyphenyl]methanesulfonamide 868408-30-4P, [5-Chloro-2-[(E)-3-[9-(4-fluorobenzyl)-3-oxa-7,9-diazabicyclo[3.3.1]non-7-yl]-3-oxopropenyl]-4-methoxyphenyl]urea 868408-32-6P, Cyclopropanecarboxylic acid N-[5-chloro-2-[(E)-3-[9-(4-fluorobenzyl)-3-oxa-7,9-diazabicyclo[3.3.1]non-7-yl]-3-oxopropenyl]-4-methoxyphenyl]amide
868408-51-9P, N-[5-Chloro-2-[(E)-3-[9-(4-fluorobenzyl)-3-oxa-7,9-diazabicyclo[3.3.1]non-7-yl]-3-oxopropenyl]-4-methylphenyl]acetamide
868408-53-1P, N-[5-Chloro-2-[(E)-3-[9-(4-fluorobenzyl)-3-oxa-7,9-diazabicyclo[3.3.1]non-7-yl]-3-oxopropenyl]-4-(pyrazin-2-yl)phenyl]acetamide 868408-54-2P, N-[5-Chloro-2-[(E)-3-[9-(4-fluorobenzyl)-3-oxa-7,9-diazabicyclo[3.3.1]non-7-yl]-3-oxopropenyl]-4-(pyridin-2-yl)phenyl]acetamide
868408-67-7P, [5-Chloro-2-[(E)-3-[(1S,5R,9S)-9-[(4-fluorophenyl)amino]-3-oxa-7-azabicyclo[3.3.1]non-7-yl]-3-oxopropenyl]-4-trifluoromethoxyphenyl]urea 868408-71-3P, N-[5-Chloro-2-[(E)-3-[(1S,5R,9S)-9-[(4-fluorophenyl)amino]-3-oxa-7-azabicyclo[3.3.1]non-7-yl]-3-oxopropenyl]-4-trifluoromethoxyphenyl]acetamide 868408-72-4P, N-[5-Chloro-2-[(E)-3-[(1S,5R,9R)-9-[(4-fluorophenyl)amino]-3-oxa-7-azabicyclo[3.3.1]non-7-yl]-3-oxopropenyl]-4-methoxyphenyl]acetamide
868547-42-6P, N-[5-Chloro-2-[(E)-3-[(1S,5R,9R)-9-[(4-fluorophenyl)amino]-3-oxa-7-azabicyclo[3.3.1]non-7-yl]-3-oxopropenyl]-4-trifluoromethoxyphenyl]acetamide 868547-44-8P, N-[5-Chloro-2-[(E)-3-[(1S,5R,9S)-9-[(4-fluorophenyl)amino]-3-oxa-7-azabicyclo[3.3.1]non-7-yl]-3-oxopropenyl]-4-methoxyphenyl]acetamide
RL: DGN (Diagnostic use); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate, neuroimaging marker; preparation of bicyclic heterocycles as CCR-1 antagonists)

RN 868408-11-1 CAPLUS

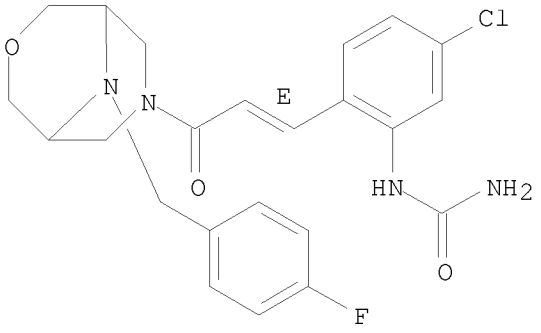
CN Acetamide, N-[5-chloro-2-[(1E)-3-[9-[(4-fluorophenyl)methyl]-3-oxa-7,9-diazabicyclo[3.3.1]non-7-yl]-3-oxo-1-propen-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



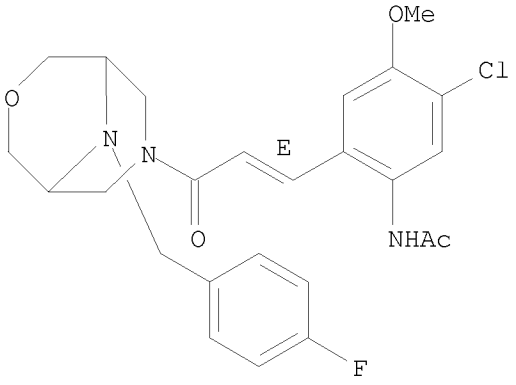
RN 868408-19-9 CAPLUS
CN Urea, N-[5-chloro-2-[(1E)-3-[9-[(4-fluorophenyl)methyl]-3-oxa-7,9-diazabicyclo[3.3.1]non-7-yl]-3-oxo-1-propen-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



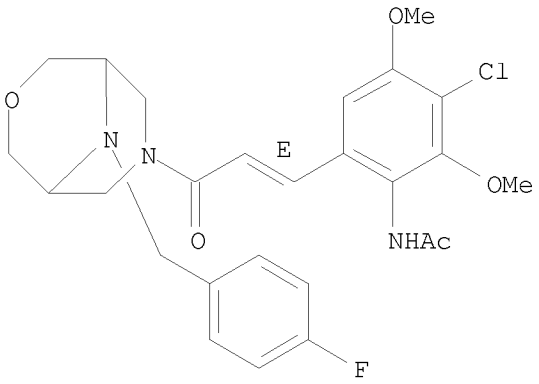
RN 868408-20-2 CAPLUS
CN Acetamide, N-[5-chloro-2-[(1E)-3-[9-[(4-fluorophenyl)methyl]-3-oxa-7,9-diazabicyclo[3.3.1]non-7-yl]-3-oxo-1-propen-1-yl]-4-methoxyphenyl]- (CA INDEX NAME)

Double bond geometry as shown.



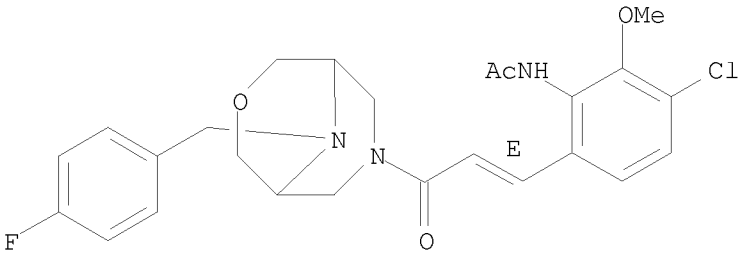
RN 868408-27-9 CAPLUS
CN Acetamide, N-[3-chloro-6-[(1E)-3-[9-[(4-fluorophenyl)methyl]-3-oxa-7,9-diazabicyclo[3.3.1]non-7-yl]-3-oxo-1-propen-1-yl]-2,4-dimethoxyphenyl]- (CA INDEX NAME)

Double bond geometry as shown.



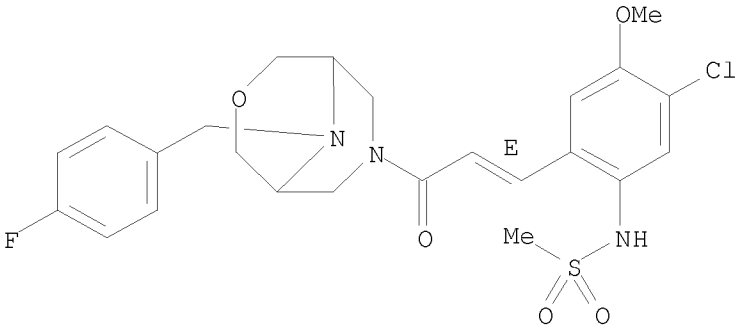
RN 868408-28-0 CAPLUS
CN Acetamide, N-[3-chloro-6-[(1E)-3-[9-[(4-fluorophenyl)methyl]-3-oxa-7,9-diazabicyclo[3.3.1]non-7-yl]-3-oxo-1-propen-1-yl]-2-methoxyphenyl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 868408-29-1 CAPLUS
CN Methanesulfonamide, N-[5-chloro-2-[(1E)-3-[9-[(4-fluorophenyl)methyl]-3-oxa-7,9-diazabicyclo[3.3.1]non-7-yl]-3-oxo-1-propen-1-yl]-4-methoxyphenyl]- (CA INDEX NAME)

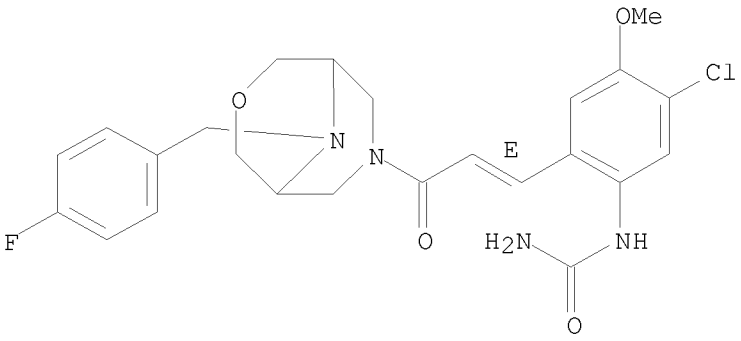
Double bond geometry as shown.



RN 868408-30-4 CAPLUS
CN Urea, N-[5-chloro-2-[(1E)-3-[9-[(4-fluorophenyl)methyl]-3-oxa-7,9-

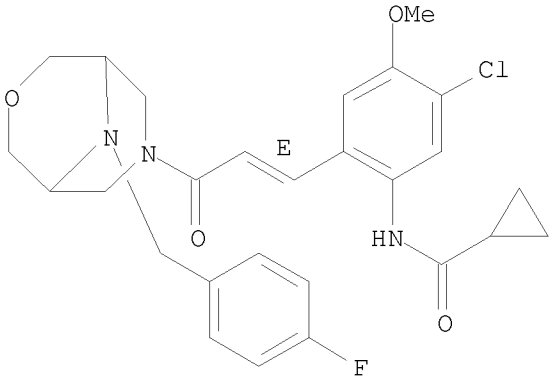
diazabicyclo[3.3.1]non-7-yl]-3-oxo-1-propen-1-yl]-4-methoxyphenyl]- (CA INDEX NAME)

Double bond geometry as shown.



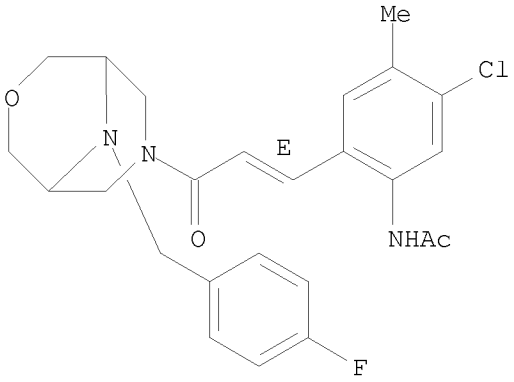
RN 868408-32-6 CAPLUS
CN Cyclopropanecarboxamide, N-[5-chloro-2-[(1E)-3-[9-[(4-fluorophenyl)methyl]-3-oxa-7,9-diazabicyclo[3.3.1]non-7-yl]-3-oxo-1-propen-1-yl]-4-methoxyphenyl]- (CA INDEX NAME)

Double bond geometry as shown.



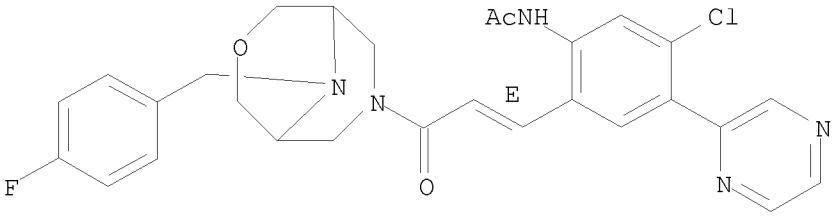
RN 868408-51-9 CAPLUS
CN Acetamide, N-[5-chloro-2-[(1E)-3-[9-[(4-fluorophenyl)methyl]-3-oxa-7,9-diazabicyclo[3.3.1]non-7-yl]-3-oxo-1-propen-1-yl]-4-methylphenyl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 868408-53-1 CAPLUS
CN Acetamide, N-[5-chloro-2-[(1E)-3-[9-[(4-fluorophenyl)methyl]-3-oxa-7,9-diazabicyclo[3.3.1]non-7-yl]-3-oxo-1-propen-1-yl]-4-(2-pyrazinyl)phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 868408-54-2 CAPLUS
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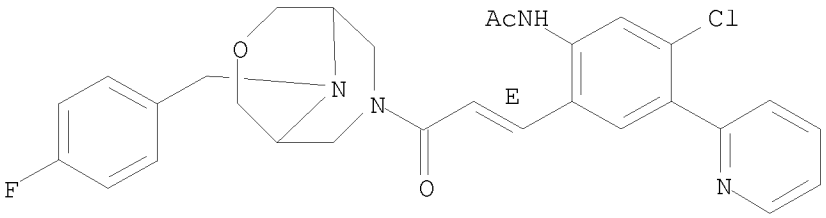
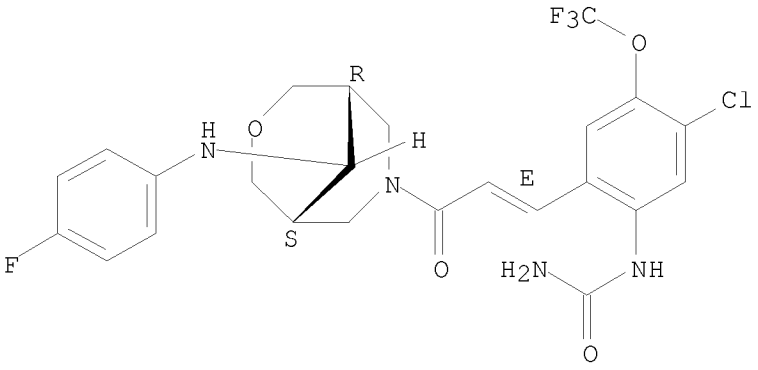
Double bond geometry as shown.



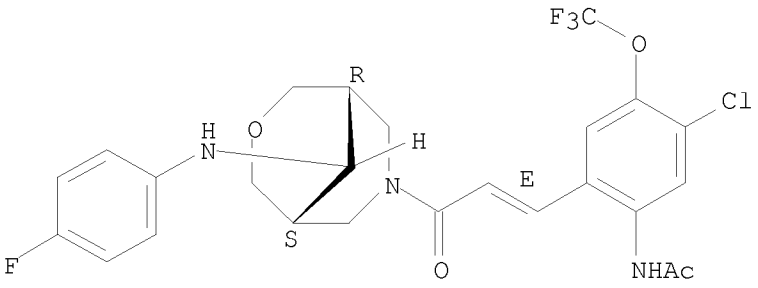
RN 868408-67-7 CAPLUS
CN Urea, N-[5-chloro-2-[(1E)-3-[(9-anti)-9-[(4-fluorophenyl)amino]-3-oxa-7-azabicyclo[3.3.1]non-7-yl]-3-oxo-1-propen-1-yl]-4-(trifluoromethoxy)phenyl]- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



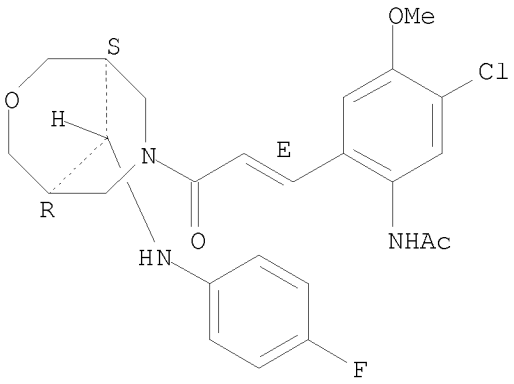
RN 868408-71-3 CAPLUS
CN Acetamide, N-[5-chloro-2-[(1E)-3-[(9-anti)-9-[(4-fluorophenyl)amino]-3-oxa-7-azabicyclo[3.3.1]non-7-yl]-3-oxo-1-propen-1-yl]-4-(trifluoromethoxy)phenyl]- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



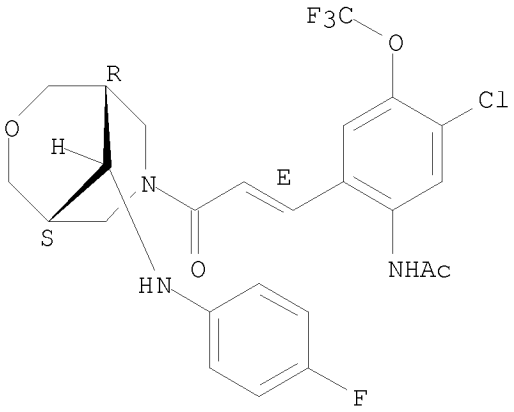
RN 868408-72-4 CAPLUS
CN Acetamide, N-[5-chloro-2-[(1E)-3-[(9-anti)-9-[(4-fluorophenyl)amino]-3-oxa-7-azabicyclo[3.3.1]non-7-yl]-3-oxo-1-propen-1-yl]-4-methoxyphenyl]- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



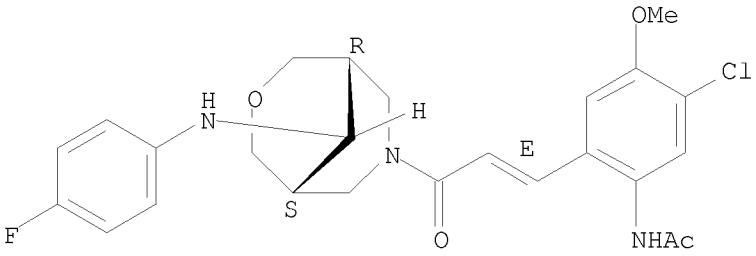
RN 868547-42-6 CAPLUS
CN Acetamide, N-[5-chloro-2-[(1E)-3-[(9-syn)-9-[(4-fluorophenyl)amino]-3-oxa-7-azabicyclo[3.3.1]non-7-yl]-3-oxo-1-propen-1-yl]-4-(trifluoromethoxy)phenyl]- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



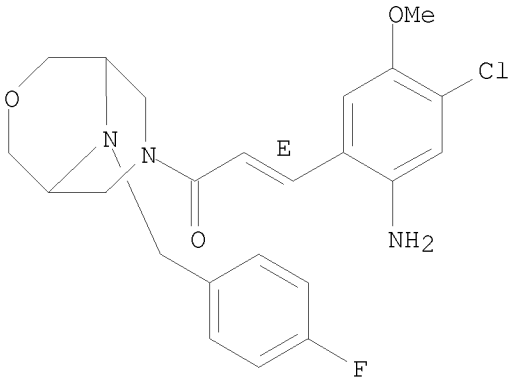
RN 868547-44-8 CAPLUS
CN Acetamide, N-[5-chloro-2-[(1E)-3-[(9-syn)-9-[(4-fluorophenyl)amino]-3-oxa-7-azabicyclo[3.3.1]non-7-yl]-3-oxo-1-propen-1-yl]-4-methoxyphenyl]- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



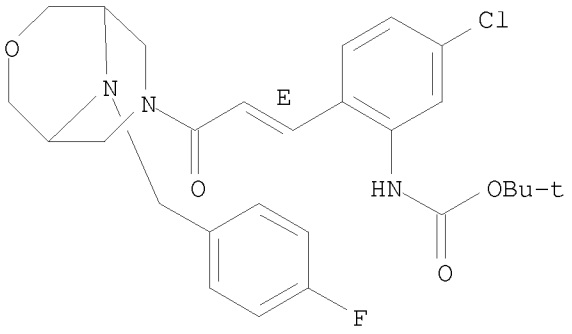
IT 868408-33-7, (E)-3-(2-Amino-4-chloro-5-methoxyphenyl)-1-[9-(4-fluorobenzyl)-3-oxa-7,9-diazabicyclo[3.3.1]non-7-yl]prop-2-enone
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of bicyclic heterocycles as CCR-1 antagonists)
RN 868408-33-7 CAPLUS
CN 2-Propen-1-one, 3-(2-amino-4-chloro-5-methoxyphenyl)-1-[9-[(4-fluorophenyl)methyl]-3-oxa-7,9-diazabicyclo[3.3.1]non-7-yl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



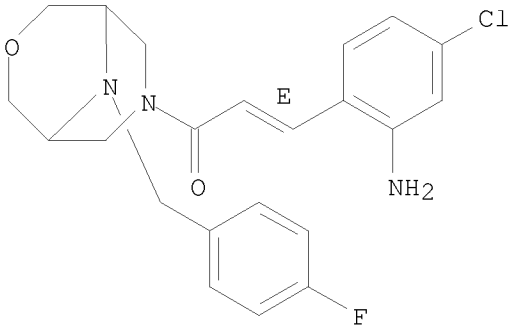
IT 868408-12-2P, (E)-[5-Chloro-2-[3-[9-(4-fluorobenzyl)-3-oxa-7,9-diazabicyclo[3.3.1]non-7-yl]-3-oxopropenyl]phenyl]carbamic acid tert-butyl ester 868408-13-3P, (E)-3-(2-Amino-4-chlorophenyl)-1-[9-(4-fluorobenzyl)-3-oxa-7,9-diazabicyclo[3.3.1]non-7-yl]prop-2-enone 868408-70-2P, (E)-3-(2-Amino-4-chloro-5-trifluoromethoxyphenyl)-1-[(1S,5R,9S)-9-[(4-fluorophenyl)amino]-3-oxa-7-azabicyclo[3.3.1]non-7-yl]prop-2-enone 868547-43-7P, (E)-3-(2-Amino-4-chloro-5-trifluoromethoxyphenyl)-1-[(1S,5R,9R)-9-[(4-fluorophenyl)amino]-3-oxa-7-azabicyclo[3.3.1]non-7-yl]prop-2-enone
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of bicyclic heterocycles as CCR-1 antagonists)
RN 868408-12-2 CAPLUS
CN Carbamic acid, [5-chloro-2-[(1E)-3-[9-[(4-fluorophenyl)methyl]-3-oxa-7,9-diazabicyclo[3.3.1]non-7-yl]-3-oxo-1-propenyl]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



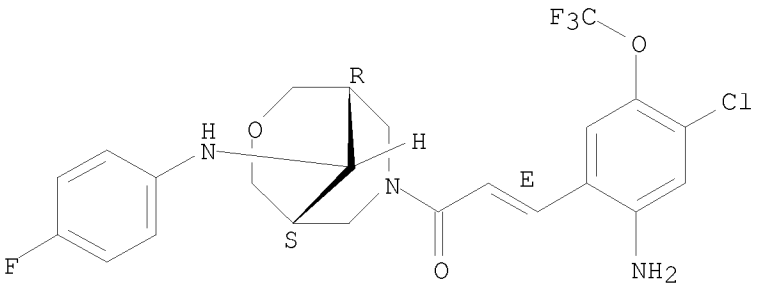
RN 868408-13-3 CAPLUS
CN 2-Propen-1-one, 3-(2-amino-4-chlorophenyl)-1-[9-[(4-fluorophenyl)methyl]-3-oxa-7,9-diazabicyclo[3.3.1]non-7-yl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 868408-70-2 CAPLUS
CN 2-Propen-1-one, 3-[2-amino-4-chloro-5-(trifluoromethoxy)phenyl]-1-[(9-syn)-9-[(4-fluorophenyl)amino]-3-oxa-7-azabicyclo[3.3.1]non-7-yl]-, (2E)- (CA INDEX NAME)

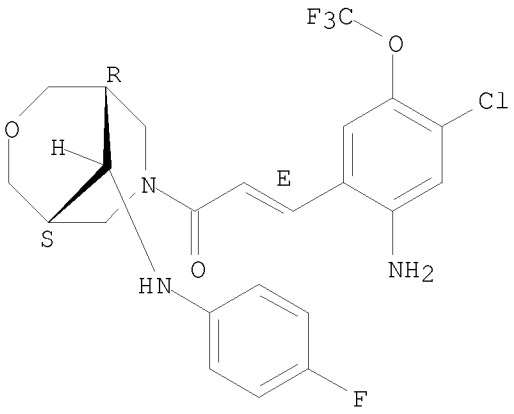
Relative stereochemistry.
Double bond geometry as shown.



RN 868547-43-7 CAPLUS
CN 2-Propen-1-one, 3-[2-amino-4-chloro-5-(trifluoromethoxy)phenyl]-1-[(9-anti)-9-[(4-fluorophenyl)amino]-3-oxa-7-azabicyclo[3.3.1]non-7-yl]-, (2E)-

(CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



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